

# Chemoinformatics of Ionic Liquids and Solids

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## Introduction

The **Chemical Property Viewer (CPV)** is an open-access portal to data of molecular and ionic compounds. The accessible data sources currently include the **ThermoML** Archive and *Axeleratio's* information snippets.

CPV implements a simple search flow: **CPV Home -> Search -> Select -> View -> Fork.**

The **View** page displays data and/or brief annotations of compound-related information. The user may “**fork**” to the associated abstracts (and full papers, typically for subscribers only) via the **Document Object Identifier (DOI)** or to the ThermoML source files.

CPV supports search requests with chemist-friendly input options for **chemical identifiers** including chemical compound names (synonyms, acronyms), **compound class identifiers** (names, structural notations), registry numbers, and compositional or (semi-)structural formulae. Ionic compounds can be searched by **cation-anion input**. Search methods via **ion classes** are also provided.

Here, we demonstrate and explain the abstraction of chemical names and structures using **XML Topic Maps (XTM)** as the central representation of chemical identifiers. Further, the XTM representation of **associations** such as **salt/ionic-components relations** and **chemical/chemical-class relations** are discussed.

## Search Example

The screen shots show the search sequence for **1-benzyl-3-methylimidazolium chloride**.

### Search:

The **cation class notation**, **1R3BzIM** (1-alkyl-3-benzylimidazolium cation), and the **anion class name**, **halogenide**, has been entered.

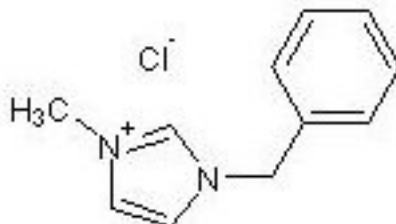
### Select:

Some salts that meet the search criteria have been found. Typically such a selection set is a result of using **ionic class names/notations**, or **stoichiometric formulae** for which various isomeric compounds are possible.

### View:

A referenced annotation regarding the **pyrolysis of 1-benzyl-3-methylimidazolium chloride** the has been located and displayed.

The example illustrates CPV's versatility in supporting users with **diverse preferences of chemical/structural nomenclature**.



# CPV Home at

<http://www.axeleratio.com/cpv>



## Chemical Property Viewer

The Chemical Property Viewer (CPV) is designed to find, browse, view and compare property data of chemical substances, mixtures, and materials. Goal of the CPV Project is to provide free, quick-by-click, and informed access to chemical information that supports advanced material science and sustainable chemistry.

### Info & News

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- :: [Data scope](#)

### ThermoML

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### Ionic Liquids

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### Literature

- :: [EnviroInfo2007 Paper](#)

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### Contact

- :: Axel at [axeleratio@yahoo.com](mailto:axeleratio@yahoo.com)

Customize: [Temperature](#) [Pressure](#)

### Select ThermoML-Archive substance by

- [Inorganic compound name](#)
- [Organic compound name](#)
- [CAS registry number](#)
- [Molecular formula](#)

### Special substances and materials

- [Ionic liquids and solids](#)

### Chemical Species

- [Cation](#)
- [Anion](#)

## Search:

<b>How to find salts?</b> <p>Use the <b>input form on the right</b> to find salts by their cation-anion composition. The info boxes below describe various options to specify <b>ions</b> and <b>ion classes</b> and assist you in applying <b>short ion notations</b> to minimize your typing needs depending on the targeted salt.</p>	<b>Salt Ions</b> Cation: <input type="text" value="1R3BzIM"/> Anion: <input type="text" value="halogenide"/>  <input type="button" value="Submit"/> <input type="button" value="Reset"/>					
<b>Search example</b> <b>1-butyl-3-methylimidazolium chloride</b>  Options to identify ions: <table><tr><td>Cation:</td><td>Anion:</td></tr><tr><td>1-butyl-3-methylimidazolium 1Bu3MeIM C8H15N2 80432-08-2</td><td>chloride Cl 16887-00-6</td></tr></table>	Cation:	Anion:	1-butyl-3-methylimidazolium 1Bu3MeIM C8H15N2 80432-08-2	chloride Cl 16887-00-6	<b>Names of specific ions</b>  Ion names are entered with lower-case letters:  <b>1,3-dimethylimidazolium</b> <b>diphenyliodonium</b> <b>p-toluenesulfonate</b> <b>tetrafluoroborate</b>  Exceptions include names that contain atomic symbols:  N-butylpyridinium N,N-diethyl-N-(1-methylethyl)-2-propanaminium O,O-diethylthiophosphate	<b>Metal cations and metal-containing anions</b>  Metal cations can simply be entered by their element name or symbol. Metal cations in a particular oxidation state are specified by additionally typing the oxidation state in roman numerals enclosed in parenthesis, for example <b>Cu(I)</b> or <b>Cu(II)</b> . Metal-containing anions are specified in a similar way or shorter by formula:  <b>tetrachloroplatinate(II)</b> or <b>PtCl4</b> <b>hexachloroplatinate(IV)</b> or <b>PtCl6</b> <b>hexabromosmate(IV)</b> or <b>OsBr6</b> <b>perrhenate(VII)</b> or <b>ReO4</b>
Cation:	Anion:					
1-butyl-3-methylimidazolium 1Bu3MeIM C8H15N2 80432-08-2	chloride Cl 16887-00-6					
<b>Short notations and acronyms</b>  For the <b>bis[(trifluoromethyl)sulfonyl]imide</b> anion, use the shorter notations <b>NTf2</b> or <b>Tf2N</b> . Use acronyms:  <b>BMIM</b> for 1-butyl-3-methylimidazolium <b>MMIM</b> for 1,3-dimethylimidazolium  Further details:  <a href="#">Short notations for organic cations</a> <a href="#">Short notations for organic anions</a>	<b>Names of ion classes</b>  Salts are also searchable by entering ion class names or codes for cations and anions such as <b>alkali</b> and <b>halogenide</b> . Further examples:  tetraalkylammonium or R4N 1-alkylpyridinium or 1RPY 1,3-dialkylimidazolium or 1R3RIM or R2IM 1,1-dialkylpyrrolidinium or 1R1RPL alkoxyethylsulfate or ROCH2CH2OSO3  Details: <a href="#">Organic cation classes</a>   <a href="#">Organic anion classes</a>	<b>More ion notations and identifiers</b>  CAS Registry Numbers for ions:  <a href="#">CASRNs for cations</a> <a href="#">CASRNs for anions</a>				

## Select:



### Chemical Property Viewer: Ionic Liquids and Solids

[Home](#) > [Search](#) > [Select](#)

Select from the following salts that match your query [1R3BzIM][halogenide]:

- 1-benzyl-3-methylimidazolium chloride
- 1-benzyl-3-methylimidazolium bromide
- 1-benzyl-3-methylimidazolium iodide
- 1-benzyl-3-ethylimidazolium iodide

View:



Chemical Property Viewer: Ionic Liquids and Solids

[Home](#) > [Search](#) > [Select](#) > View

## 1-benzyl-3-methylimidazolium chloride

$[\text{C}_{11}\text{H}_{13}\text{N}_2]^{1+}[\text{Cl}]^{1-} \mid \text{C}_{11}\text{H}_{13}\text{ClN}_2 \rightarrow \text{M}=208.69$

### Table of Search Results

[Stability & Reactivity](#)

### Stability & Reactivity

**Pyrolysis:** 1-benzyl-3-methylimidazolium chloride decomposes into 1-methylimidazole and 1-benzylimidazole (ratio: 1:0.67) and the corresponding organyl chlorides. (over a period of 0.5-1.5 h at 220-260 °C with a pressure below 2 mm) [2]<sup>o</sup>

[1] Benedict K. M. Chan, Nyuk-Hon Chang and M. Ross Grimmitt: The Synthesis and Thermolysis of Imidazole Quaternary Salts, *Aust. J. Chem.* 1977, 30, 2005-2013. | DOI: [10.1071/CH9772005](https://doi.org/10.1071/CH9772005)

[2] Table 1 on page(s) 2007 in [1]

# Behind the Scenes: XML

## **Search requests in CPV are answered by directly employing data from XML files.**

The CPV service uses PHP methods to load XML files, to extract and transform data, and to generate user-friendly output for display by a browser.

## **Identification of ions and compounds**

Chemical identification is supported by XML-encoded chemical dictionaries derived from XTM files organizing same-chemical identifiers, class memberships and, in the case of ions, associated electric charge information. Our **Ionic Identification XTM (IIXTM)** base currently includes over 700 ion files and 1300 salt files. Each salt files represents one ionic compound with <variant> nodes for chemical synonyms, registry numbers, structural notations and formulae and <association> nodes to relate the salt to its cation and anion components.

## **Physicochemical property data from ThermoML**

The **open-access ThermoML Archive**, maintained by the Thermodynamic Research Center (TRC) at the National Institute of Standards and Technology (NIST), contains XML files with experimental thermophysical and thermochemical property data for pure compounds and mixtures thereof. The data are published in peer-reviewed journals and each ThermoML file presents data of a particular journal article. Currently, property data for about 60 **ionic liquids** are available in the archive and can be viewed via CPV as a function of temperature and pressure depending on a particular property. (CPV also accesses over 1000 ThermoML-abstracted molecular compounds.)

## **Chemical information from XML-encoded annotations**

Whereas the current ThermoML archive is confined to five selected journals participating in the TRC/NIST effort, our XML-encoded collection of annotations is derived from a much broader spectrum of publications including journals with a defining **sustainable chemistry (green chemistry)** perspective. In addition to physicochemical data, we abstract and annotate data on safety, toxicity, electrochemistry, synthesis and potential applications including direct links (URL, **DOI**) to the reference, whenever available.

## **Quantitative Structure/Property Relationships (QSPRs)**

Chemical property estimation methods such as QSPRs for ionic compounds are based on properties and **ionic descriptors** of cations and anions. The IIXTM database facilitates testing and design of QSPRs and **ionic similarity** concepts. Currently, in-house software is developed for this purpose, using **SMILES notations** for ions in addition to IIXTM parameters. Further, **ionic order relations** are published online, which support design of **Task-Specific Ionic Liquids (TSILs)** by property-driven ion selection, for example to identify critical ions for low-melting salts:

[http://www.axeleratio.com/ip/QSPRs/order\\_ion/mpTf2N.htm](http://www.axeleratio.com/ip/QSPRs/order_ion/mpTf2N.htm) .

## References

[CPV] Drefahl, A. "Extraction and Application of Environmentally Relevant Chemical Information from the ThermoML Archive," *EnviroInfo 2007 21<sup>st</sup> International Conference on Informatics for Environmental Protection September 12-14, 2007, Warsaw, Poland*. Pages 71 to 78 in Volume 1: Plenary and session papers. Shaker Verlag GmbH, D-52018 Aachen.

Paper: <http://www.axeleratio.com/EnviroInfo2007/paper.doc>

Home: <http://www.axeleratio.com/cpv>

Salts: <http://www.axeleratio.com/cpv/salts/saltForm.php>

Cations: <http://www.axeleratio.com/cpv/cations/cationForm.php>

Anions: <http://www.axeleratio.com/cpv/anions/anionForm.php>

[ILThermo] <http://ilthermo.boulder.nist.gov/ILThermo/mainmenu.uix>

[ThermoML] <http://trc.nist.gov/ThermoML.html>

[XTM] Park, J. (Ed.) "XML Topic Maps" Addison-Wesley, Boston, 2003.